



Molecular Dynamics Simulations of Supercritical Jet Mixing

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Introduction

- High pressure heterogeneous combustion systems typically operate trans- or supercritical
 - Liquid rocket engines
 - Gas turbine combustors
 - Diesel engines
- Quantitative assessments or validated theories characterizing propellant injection at near and supercritical conditions are currently limited



Vulcain



SSME

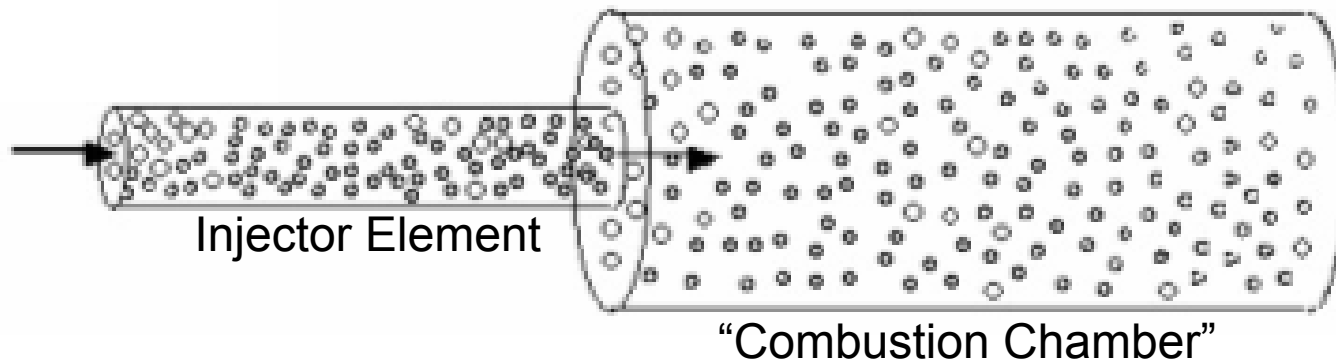


Introduction

- Because these systems operate at near and supercritical conditions, it is difficult to model the injection, mixing, atomization, and vaporization using traditional CFD
 - System becomes fully 3-D
 - Material and transport properties change significantly
 - Moves from 2-phase to 1-phase
 - Complex mixture effects

Introduction

- This research attempts to address these limitations through the use of MD as an alternate simulation tool
- Diatomic liquid nitrogen (N_2) is simulated as a non-reacting substitute to other diatomic cryogenic liquid propellants/oxidizers, i.e. H_2 or O_2
Experimental database exists
- The simulation consists of two cylinders
 - Smaller diameter cylinder representing one injector through which simulated liquid nitrogen flows
 - Larger diameter cylinder of gaseous nitrogen into which the simulated





Introduction

■ Advantages of the MD model:

- ☐ Based purely on first principles ($F=ma$)
- ☐ Can theoretically span all conditions; no need to track phase boundaries
- ☐ Geometric assumptions do not need to be made
- ☐ Equation of state, material and transport properties are not needed, and *can actually be* calculated outputs
- ☐ Mixture effects automatically incorporated



Fundamental Concepts of MD

- Dynamics of interest is contained within solution to the classical N-body problem
- MD is a numerical tool used to solve Newton's Laws of Motion, applied to motions of individual atoms or molecules
 - $F = ma$ is the only equation to solve
 - Forces on atoms derived from interatomic potentials

Fundamental Concepts of MD

■ Lennard-Jones 12-6 Potential

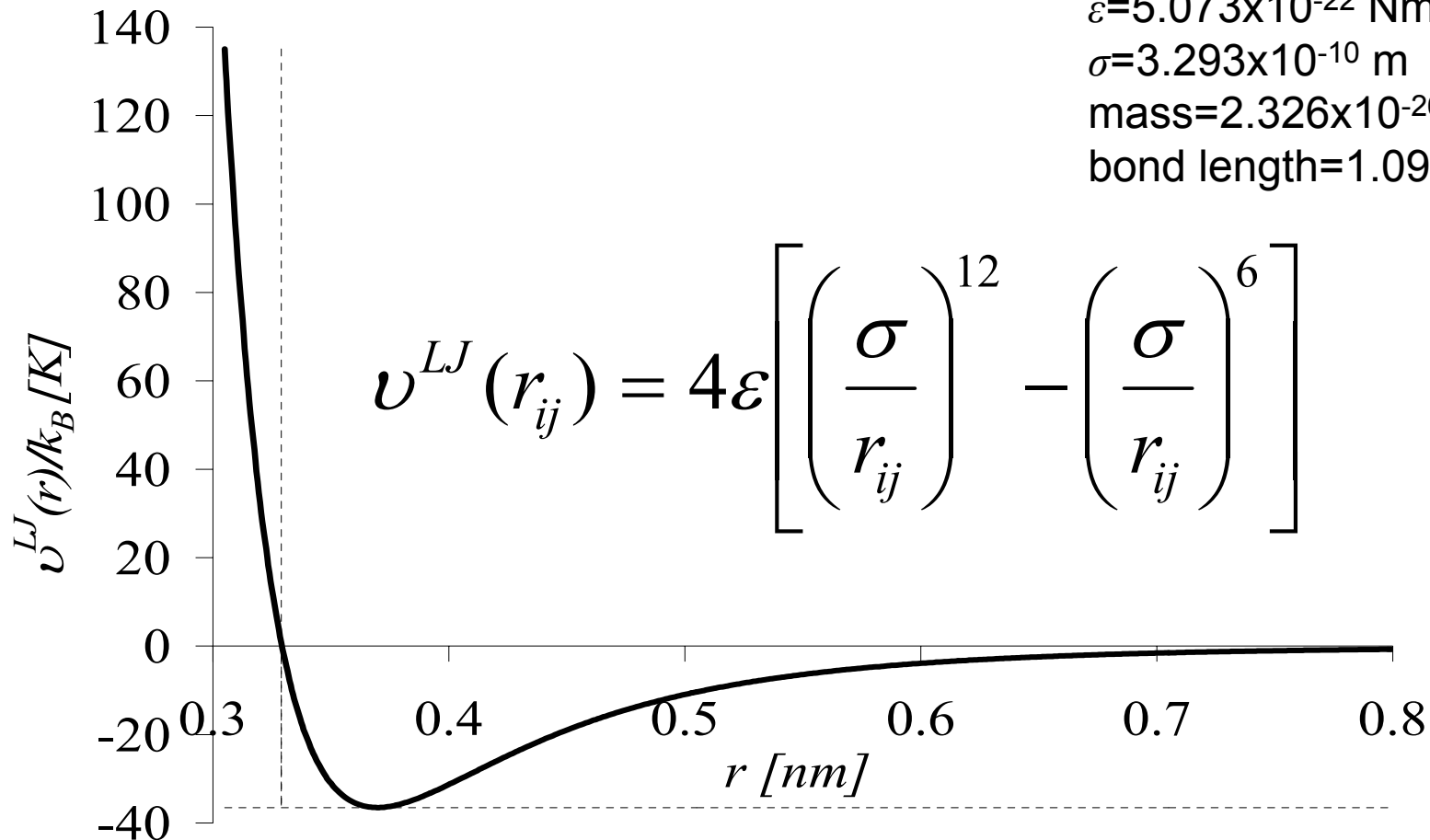
For Nitrogen Atoms:

$$\varepsilon = 5.073 \times 10^{-22} \text{ Nm}$$

$$\sigma = 3.293 \times 10^{-10} \text{ m}$$

$$\text{mass} = 2.326 \times 10^{-26} \text{ kg}$$

$$\text{bond length} = 1.094 \times 10^{-10} \text{ m}$$



Fundamental Concepts of MD

- Equations of Motion

$$m_a \mathbf{a}_i = \mathbf{F}_i = \sum_{j=1}^{N_a} \mathbf{f}_{ij}$$

- For Lennard-Jones Potential

$$\mathbf{f} = -\nabla \nu^{LJ}(\mathbf{r})$$

$$\mathbf{f}_{ij} = \left(\frac{48\varepsilon}{\sigma^2} \right) \left[\left(\frac{\sigma}{r_{ij}} \right)^{14} - \frac{1}{2} \left(\frac{\sigma}{r_{ij}} \right)^8 \right] \mathbf{r}$$

- Solve Numerically Using Finite Difference Velocity-Verlet Algorithm

$$\mathbf{r}(t + \Delta t) = \mathbf{r}(t) + \Delta t \mathbf{v}(t) + \frac{\Delta t^2 \mathbf{a}(t)}{2}$$

$$\mathbf{v}(t + \Delta t / 2) = \mathbf{v}(t) + \frac{\Delta t \mathbf{a}(t)}{2}$$

$$\mathbf{v}(t + \Delta t) = \mathbf{v}(t + \Delta t / 2) + \frac{\Delta t \mathbf{a}(t + \Delta t)}{2}$$

Fundamental Concepts of MD

- Addition of Bond Constraint to Simulate Diatomic Nitrogen Molecule

$$r_{ab}^2 = \mathbf{r}_{ab} \cdot \mathbf{r}_{ab} = \text{constant}$$

$$\frac{d(r_{ab}^2)}{dt} = 2\mathbf{r}_{ab} \cdot \mathbf{v}_{ab} = 0$$

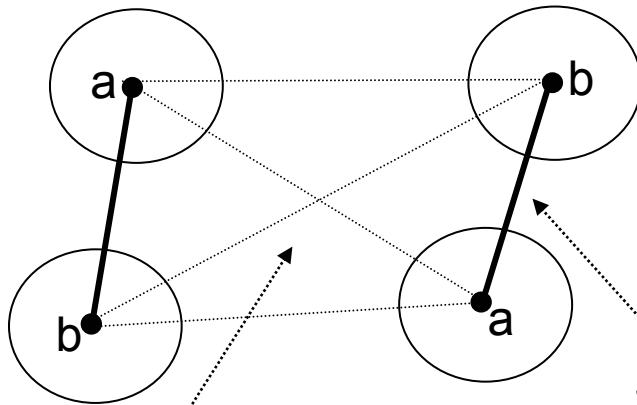
RATTLE Algorithm:

$$\mathbf{r}(t + \Delta t) = \mathbf{r}'(t + \Delta t) + \left(\frac{\Delta t^2}{2m} \right) \mathbf{g}(t)$$

$$\mathbf{v}(t + \Delta t / 2) = \mathbf{v}'(t + \Delta t / 2) + \left(\frac{\Delta t}{2m} \right) \mathbf{g}(t)$$

$$\mathbf{v}(t + \Delta t) = \mathbf{v}'(t + \Delta t) + \left(\frac{\Delta t}{2m} \right) \mathbf{g}(t + \Delta t)$$

Two N₂ Molecules:



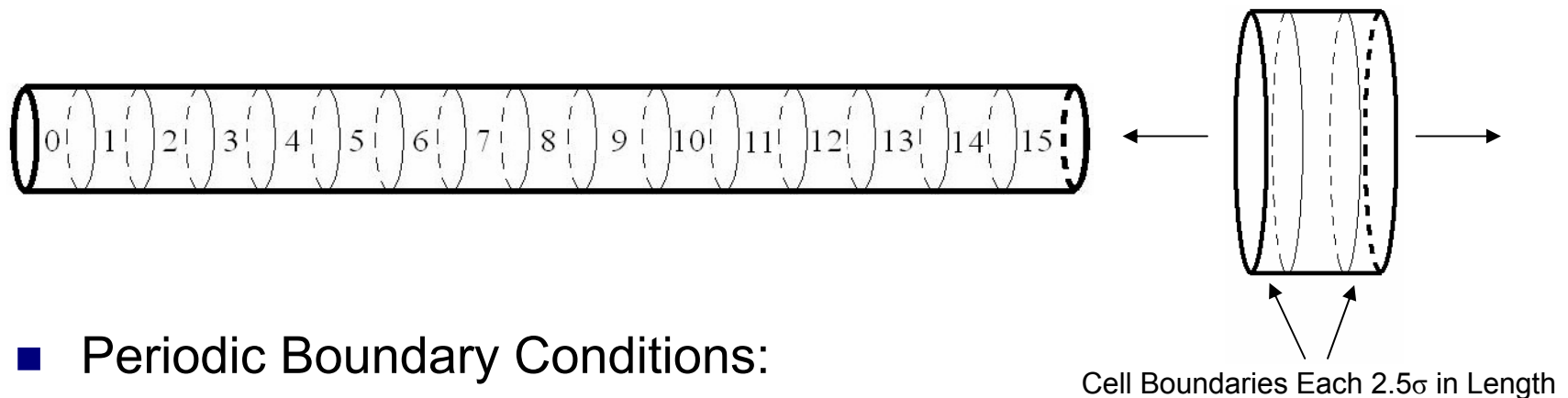
Motion of each atom in molecule simulated separately

Simulated bond using RATTLE

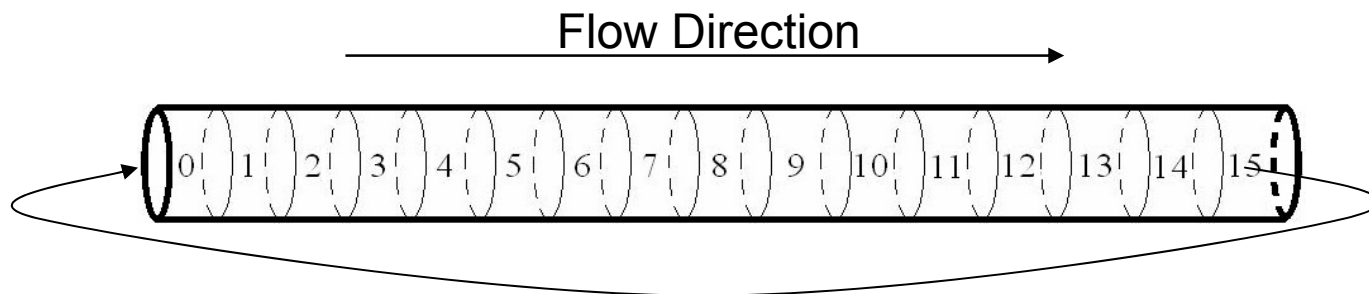
Simulation Methodology

■ Computational Domain and Processor Setup:

- Each processor assigned to handle particles within a specific geometric region
- As particles move, they are transferred between processors

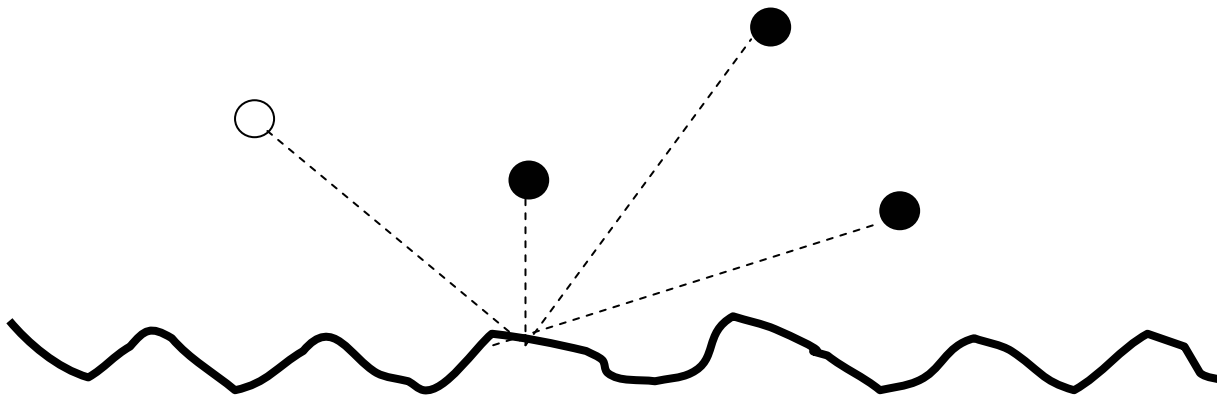


■ Periodic Boundary Conditions:



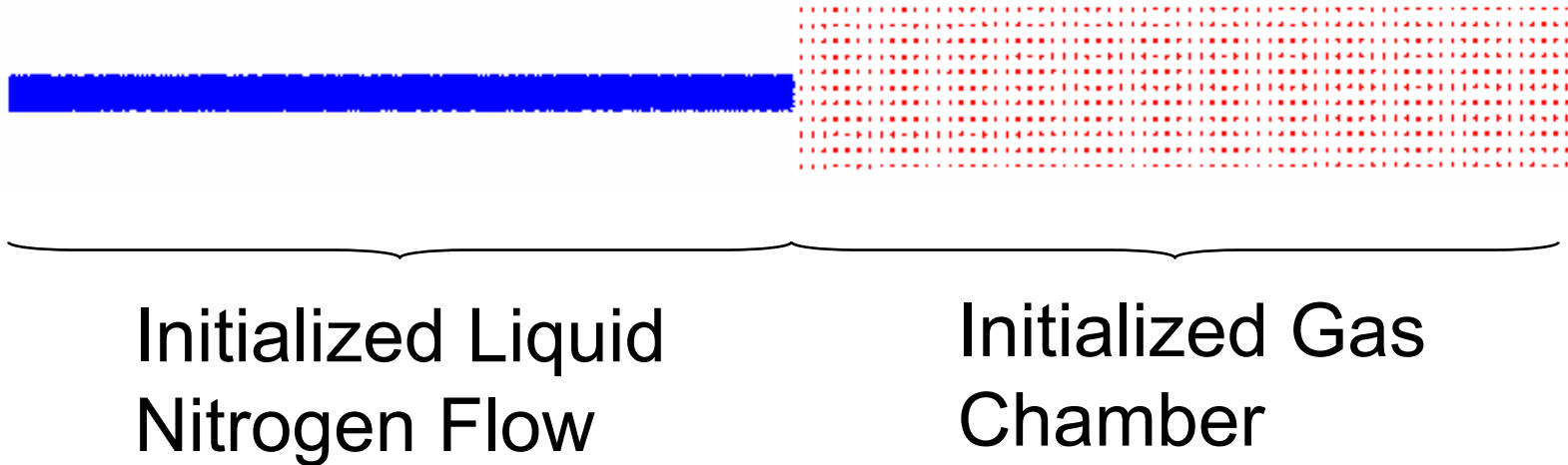
Wall Model

- Constant Temperature Wall
- Diffusely Reflecting
 - Molecules reemitted from wall in random direction with random velocity based on Maxwellian distribution scaled to the wall temperature.
 - Removes heat generated by viscous dissipation





Simulation Methodology



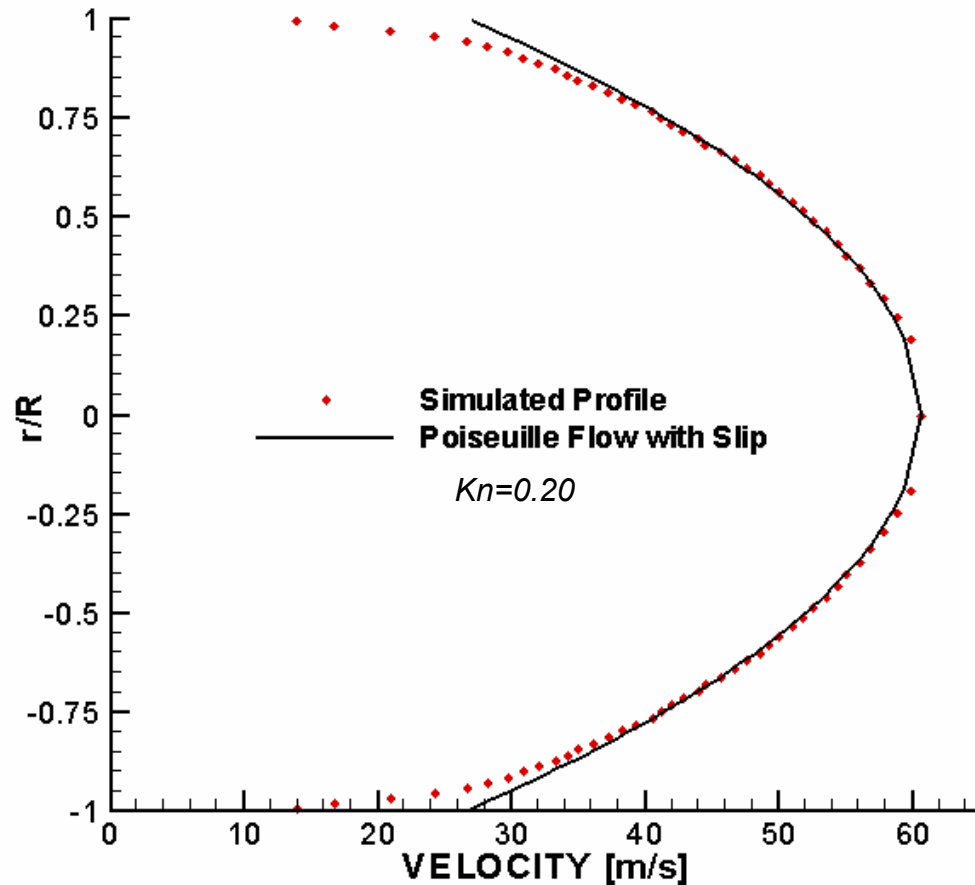
Results

■ Velocity Profile

$$\lambda = \frac{1}{\sqrt{2}\pi d^2 n} \quad Kn = \frac{\lambda}{L}$$

$$u(r) = u_{\max} - \frac{u_{\max}}{1 + 4Kn} \left(\frac{r}{R} \right)^2$$

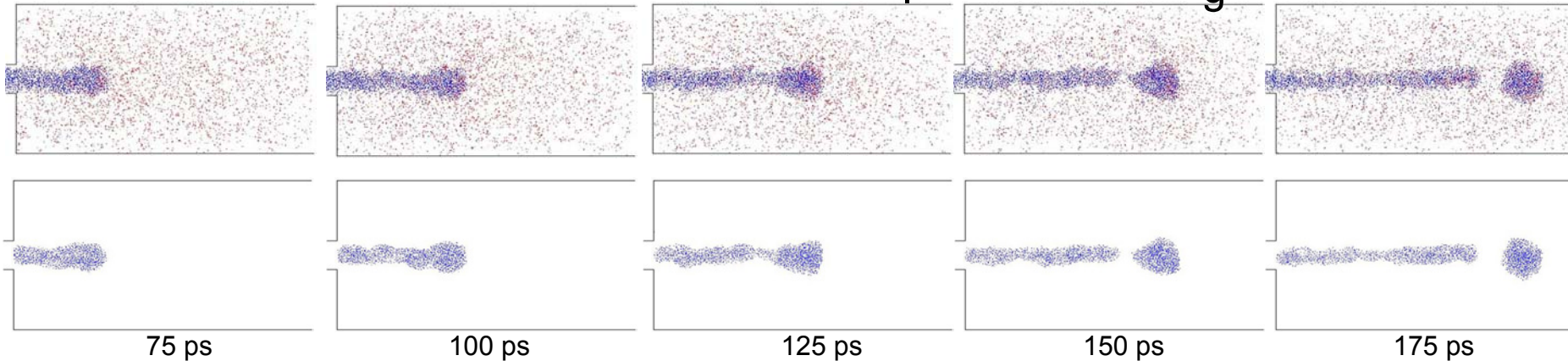
$$u(R) = -\lambda \left(\frac{du}{dr} \right)_{r=R}$$



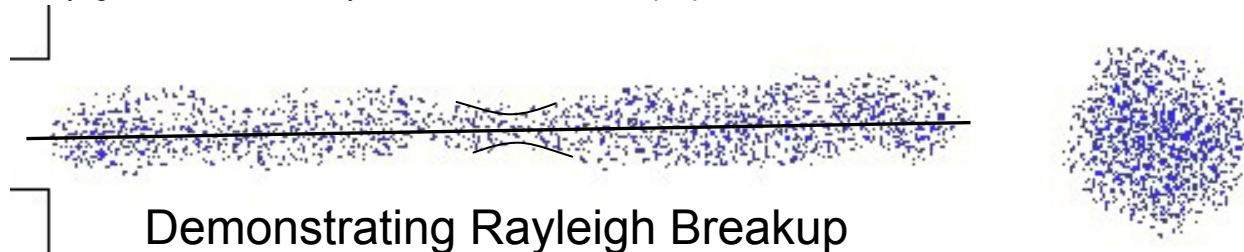
Radial Velocity Profile

Results

- 94 K, ~0.5 MPa, $Re=1.63$, $We_l=1.50$, $We_g=0.04$

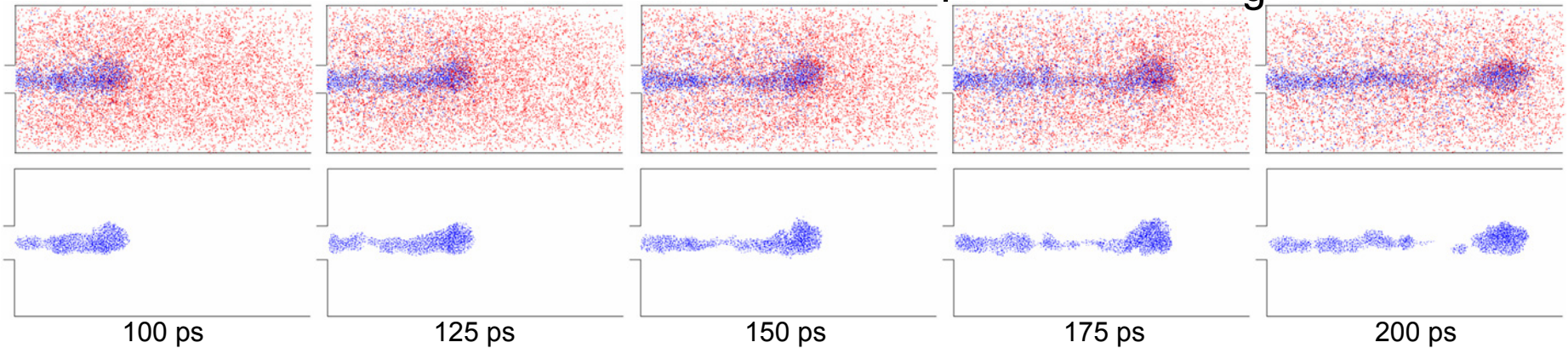


Source: Mayer, W. O., and Telaar, J., "Investigation of Breakup of Turbulent Cryogenic Variable-Density Jets." *Atomization and Sprays*, **12**, 651-666, 2002.

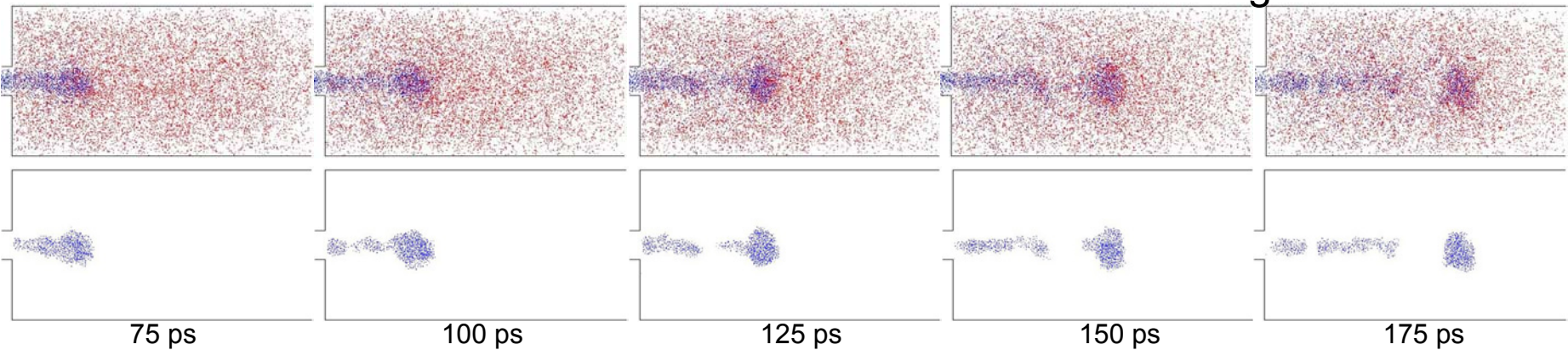


Results

■ 104 K, ~1.0 MPa, $Re=2.07$, $We_l=2.18$, $We_g=0.14$

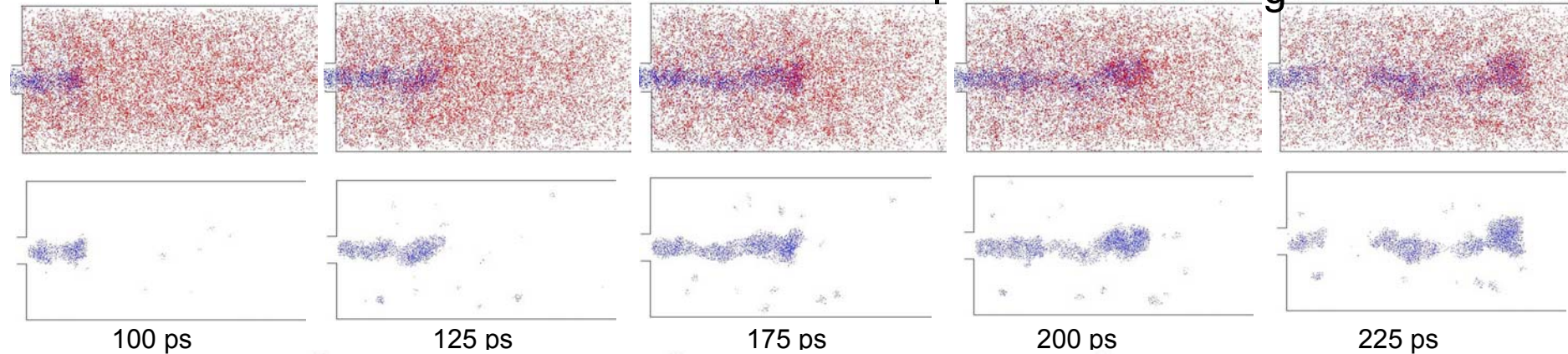


■ 114 K, ~2.0 MPa, $Re=2.71$, $We_l=4.62$, $We_g=0.45$

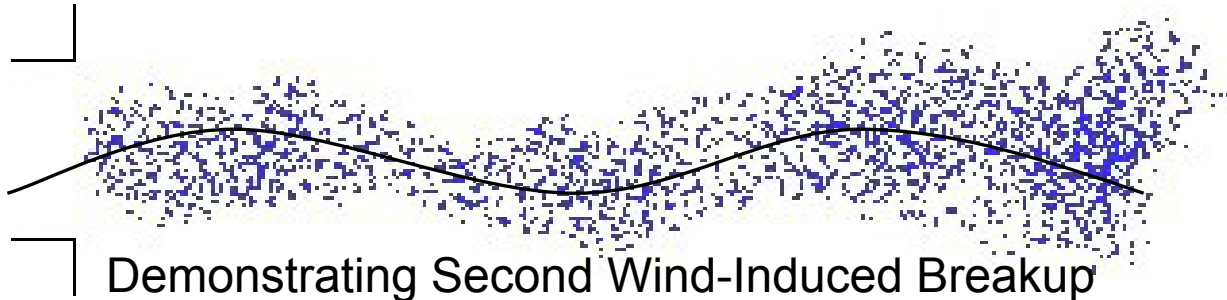


Results

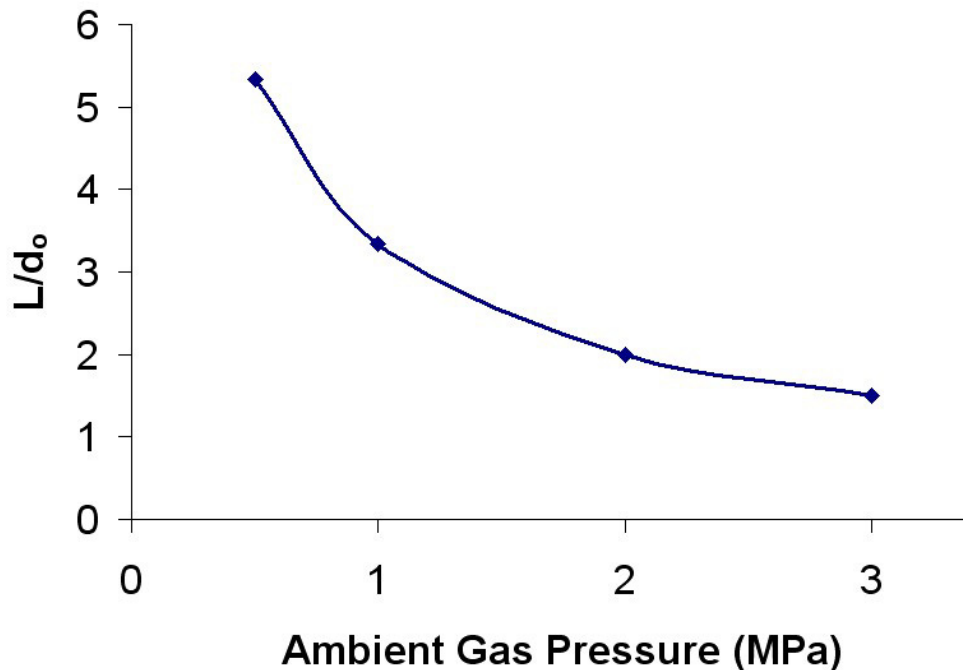
- 124 K, ~3.0 MPa, $Re=4.04$, $We_l=41.53$, $We_g=7.06$



Source: Mayer, W. O., and Telaar, J., "Investigation of Breakup of Turbulent Cryogenic Variable-Density Jets." *Atomization and Sprays*, **12**, 651-666, 2002



Results



- A decrease in breakup length with an increase in ambient pressure is observed
- The difference in breakup length between the higher ambient pressure cases is also less, indicative of higher pressures having less of an effect on breakup length

Animation

83 K

~ 0.2 MPa

$Re=1.09$

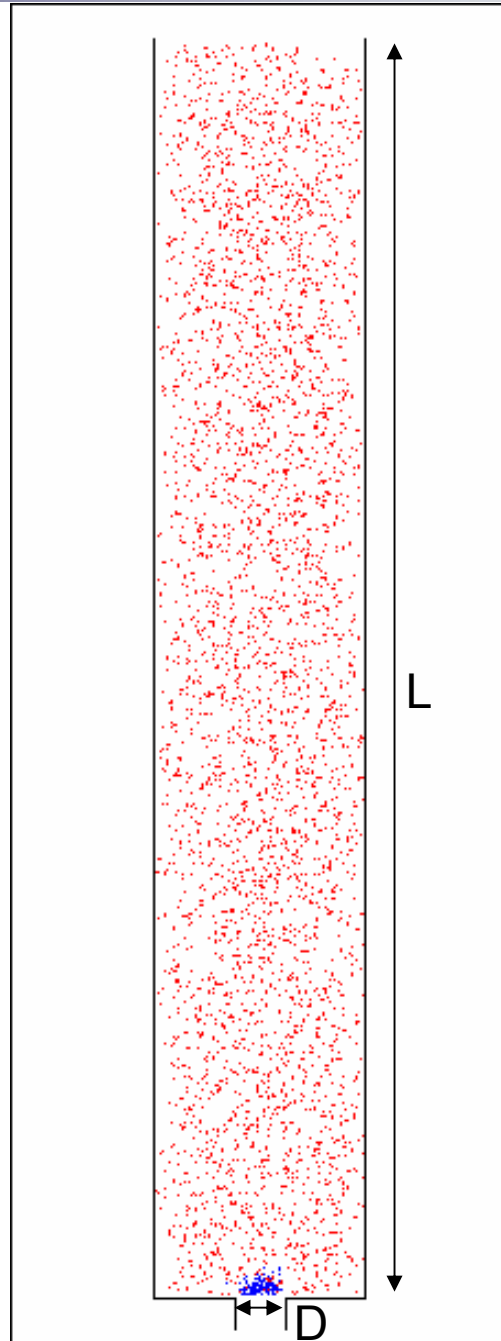
$We_l=0.84$

$We_g=0.009$

$u_{avg}=45.3$ m/s

$L/D=60$

Total Simulation Time:
1.2625 ns



Animation

83 K
~0.2 MPa

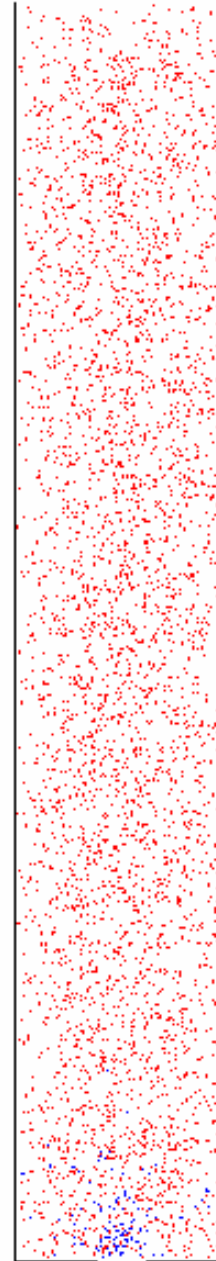
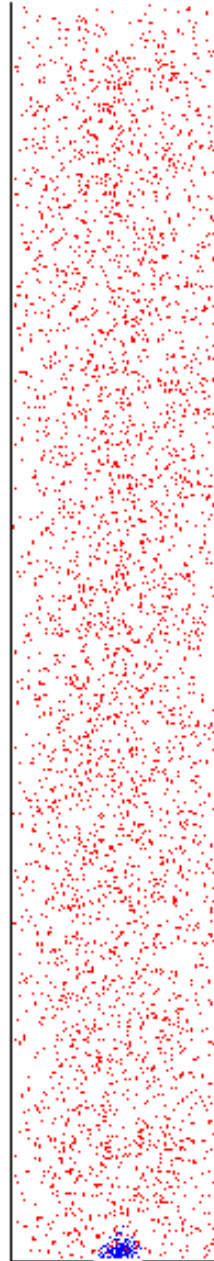
$Re=(a)0.87, (b)1.70$
 $We_l=(a)0.50, (b)1.90$
 $We_g=(a)0.005, (b)0.021$

$u_{avg}=(a)33.8 \text{ m/s}$
 $(b)66.1 \text{ m/s}$

$L/D=60$

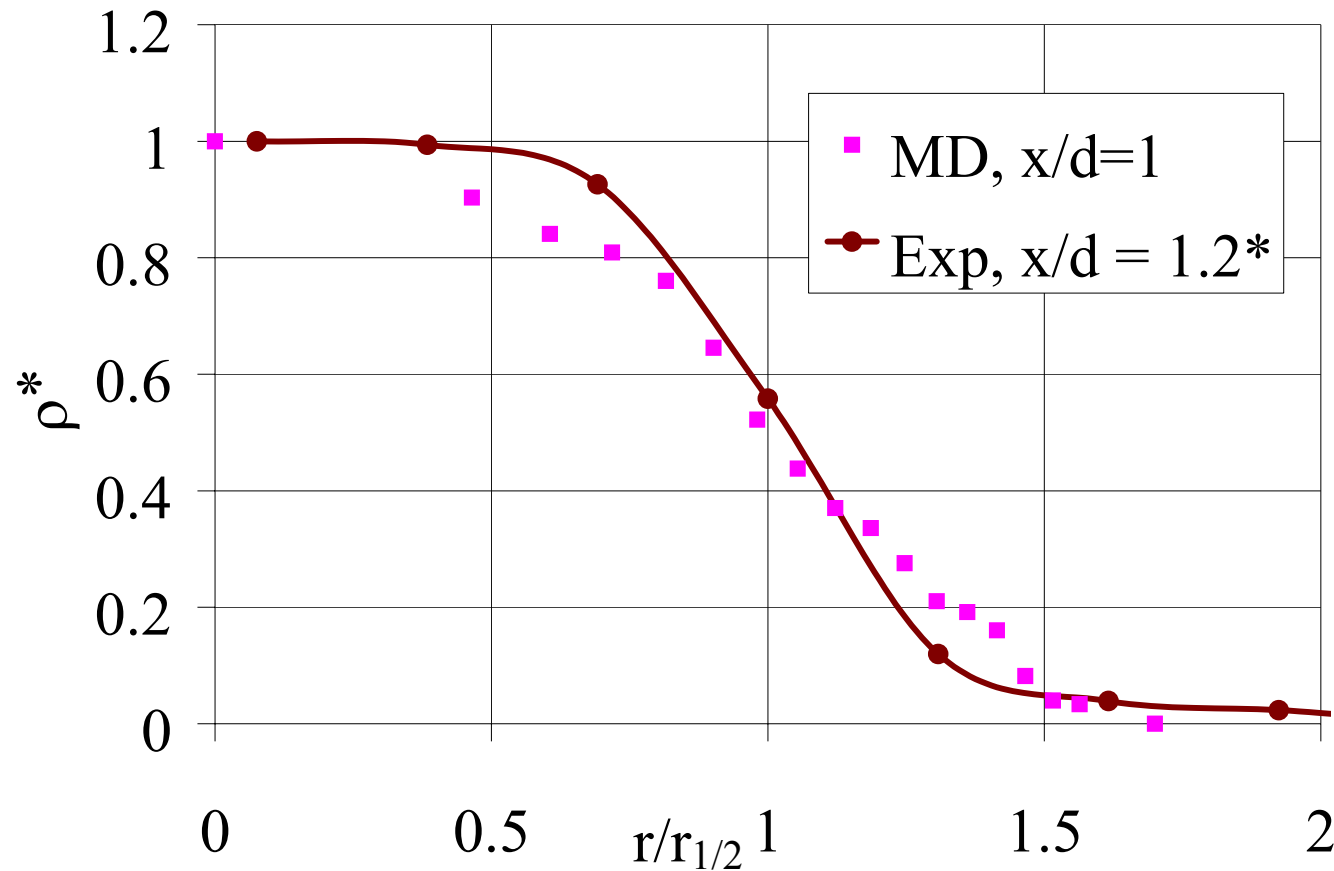
Total Simulation Time:
1.2625 ns

a



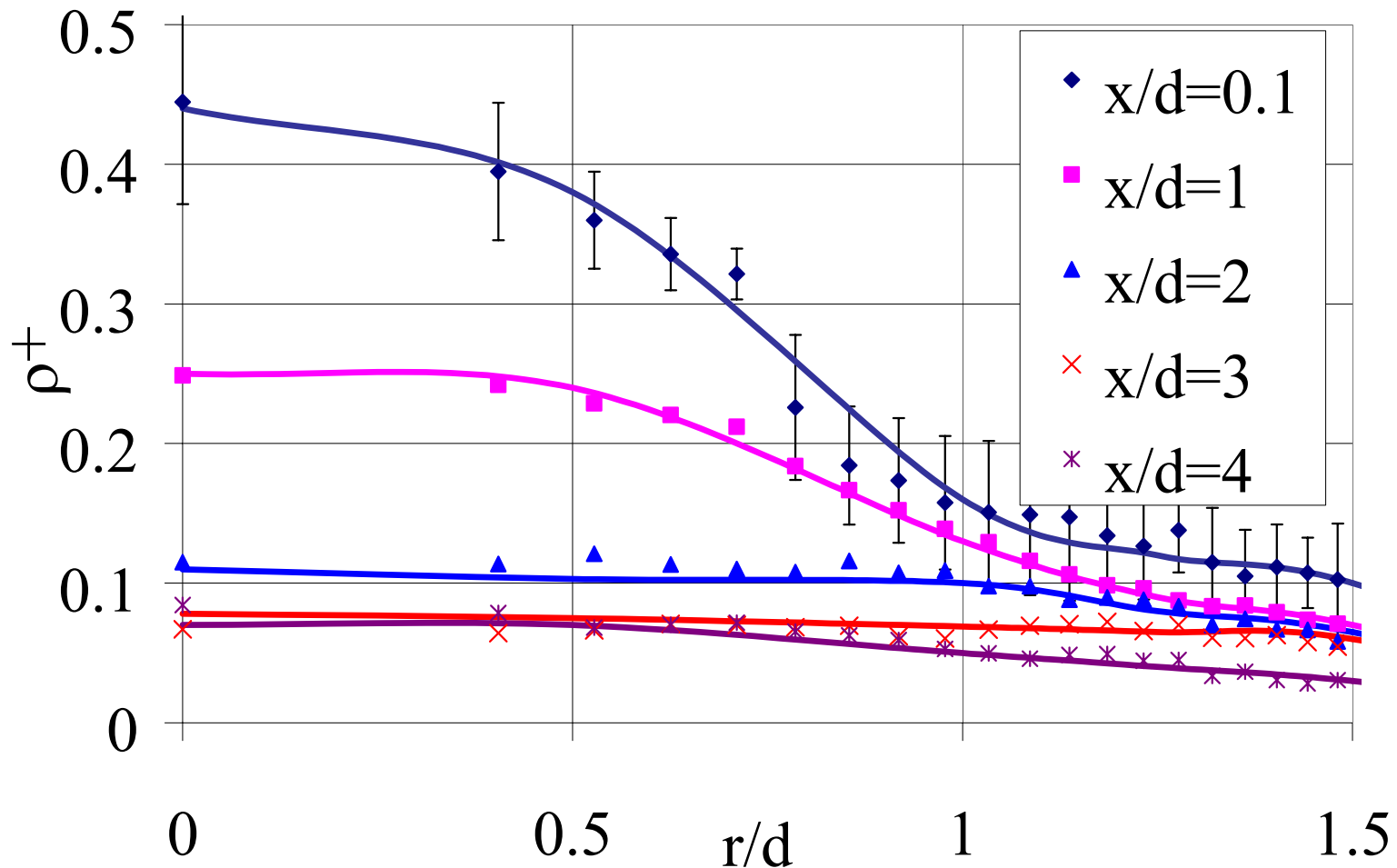
Supercritical - Comparison to Raman measurement

■ 4 MPa, 123 K



Supercritical - Computed radial density profiles

■ Target conditions, 6 MPa, 123 K, 40 m/s



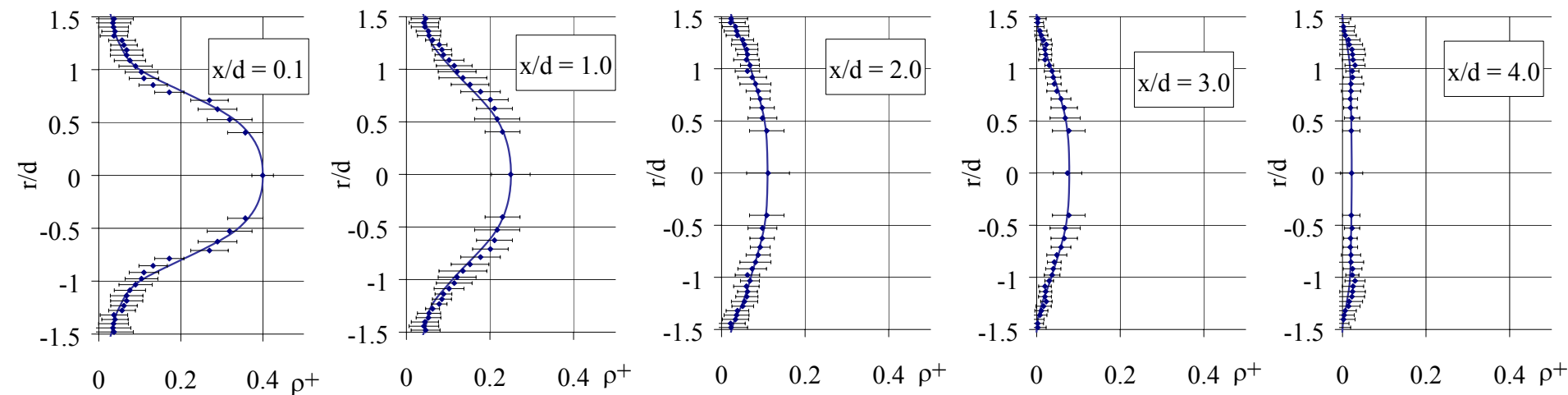
Supercritical - Evolution of computed density profiles

■ Developing Flow

□ At a given time

□ Average of five independent simulations

■ Supercritical conditions, 4 MPa, 123 K





Summary

■ Subcritical Injection Simulations:

- Rayleigh breakup is reproduced, resulting in formation of droplets due to capillary instabilities in the jet driven by surface tension
- The onset of aerodynamic effects, including the second wind-induced breakup regime, can also be seen in the cases of higher gas pressures

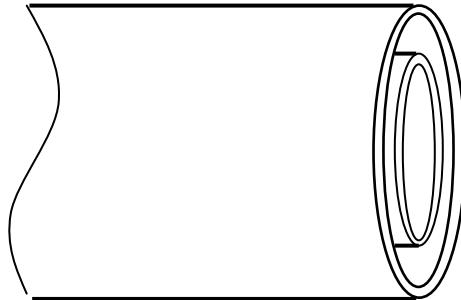


Summary (II)

- Supercritical Injection Simulations:
 - MD simulations match Raman measurements near injector exit (potential core)
 - Simulated flow still transient further downstream

Future work

- Resolve wall B.C. rotational accommodation
- Increase size of simulations
 - Generating injected particles
 - Increase tube diameter
 - Increase Re , decrease Kn
- Future work to focus more on ethanol and other hydrocarbons
- Extend geometry to include coaxial tube





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